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Biology, Sociology, Geology by Computational Physicists

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Biology, Sociology, Geology by Computational Physicists

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Erratum

Due to a technical error an old version of the advisory board for the Monograph Series on Nonlinear Science and Complexity has been printed in Volume 1 on Biology, Sociology, Geology by Computational Physicists.

On the reverse of this sheet page ii is reprinted correctly.

The Publisher

Preface

Physicists pretend not only to know everything, but also to know everything better. This applies in particular to computational statistical physicists like US. Thus many of our colleagues have applied their computer simulation techniques to fields outside of physics, and have published sometimes in biological, economic or sociological journals, and publication flow in the opposite direction has also started.

If one sets plates, knives, and forks onto a dinner table, one has to put in human organisation to order the pieces properly. The magnetic atoms in iron, on the other hand, order their magnetic orientation parallel to each other (over small distances) by themselves, and similarly water molecules in vapour cluster all by themselves into small drops when it rains. Such effects are called “self-organisation” (or “emergence”) and are typical for “complex systems” of many simple elements, often different from each other, which altogether generate effects which cannot be seen from the properties of a single element. The whole is not the simple superposition of its many parts. 65 years after van der Waals wrote his thesis with what may be regarded as the first theory to explain self-organisation in complex systems, computers became available and simulations on them triggered the systematic research activity on this field. These studies flourished during the last few decades.

Many other natural phenomena outside physics are related to the terms “complexity”, “emergence”, etc., in particular, evolutionary dynamic systems, where a population of agents evolves in time, the behaviour of each influencing the behaviour of others. Biological evolution through natural selection is the master example, but the same general concepts apply also to distant subjects, such as the occurrence of earthquakes. Other examples can be seen in diverse social behaviour and human activities such as the distribution and evolution of languages, elections, the diffusion of opinion, terrorism, etc.

The present book reviews selected applications to evolutionary biology (Chapters 3 and 4), social sciences (5 and 6) and geosciences (7), while Chapter 2 explains the general concepts of evolutionary dynamical systems, and why computer simulations of agent-based-models are the basic tool for these studies. The book as a whole is intended for graduate students and researchers not only in physics. No deep knowledge concerning the many different subjects or computer programming is required to follow the book, which can therefore be useful (we hope) to a wide and general audience. The parts we marked with asterisks con-

tain mostly additional information, not fundamental for the comprehension of the book as a whole.

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Introduction

Computational Physics is now a multidisciplinary line of research. A long time ago, it was not like that, computers were used by physicists only in order to solve classical problems resistant to the analytical approach: One is able to model the problem at hands through, say, a set of coupled differential equations, but the analytical solution for these equations is not available. The solace is the numerical solution, and the old branch of Computational Physics consists in providing fast and precise numerical methods to be applied to these cases.

Some systems, however, resist even to this numerical strategy, for instance the life cycle of a bacterium with 10 thousand proteins, a rather “simple” biological organism. The concentration of each protein varies in time according to the current concentrations of the others, and also to external stimuli. Suppose one models how each concentration depends on all others by writing down a set of 10 thousand coupled differential equations, which depend also on the possible external stimuli. Furthermore, suppose one is able to solve this mathematical problem on a computer, within a reasonable time: then, one can run the program for a given set of initial concentrations and external stimuli. In order to study the behaviour of this “simple” system, one would need to run the program again and again, for different conditions, and try to extract some useful information. Some particular stimulus may result in some particular behaviour, if it occurs when the concentration of some particular protein is high. Has it the same effect when this concentration is low? Does it depend on the concentrations of other proteins? Is the effect of two superimposed stimuli obtained simply by adding the individual effects of each one? How long does one need to wait, after the onset of some stimulus, in order for the system to have reached a state in which a renewed triggering of the stimulus would generate the same effect anew? How does this waiting time depend on the concentrations? This is an endless approach, which in some very lucky cases may be circumvented by a reductionist reasoning: to consider only the effect of some dozen proteins and stimuli, forgetting all the rest. Beyond a simple bacterium, the reader can imagine the mess one reaches in the study of a bacterial colony. Also, even worse than a 10 thousand protein life cycle is a system for which there are no fundamental equations relating the various important quan-

tities. Biological evolution, where there is no Darwin equation, is an example. Social behaviour within a human population is another, as well as the dynamics of economics. Normally, one cannot even model such a system by a set of coupled differential equations.

An alternative is population dynamics: one keeps on the computer memory the current features of each individual, and simulates the whole dynamic evolution by programming the interaction rules governing the influences of these individuals on each other, as well as external stimuli. A crucial ingredient is randomness, which is included through the use of some pseudo-random number generator. The long-term evolution of the same system is repeated many times, for different randomness and initial conditions, and averages are taken at the end. Besides the numerical solution of equations, this simulational approach is the second, modern branch of Computational Physics, introduced by the pioneering work of Metropolis, Rosenbluth, Rosenbluth, Teller and Teller (1953) half a century ago. First applied to equilibrium models of Statistical Physics, simulations are now applied to many different problems outside physics and out of equilibrium. The reason for this success is a subtle concept known as universality, discovered within the study of critical phenomena where the simulational approach has a fundamental position.

Equilibrium critical phenomena occur in macroscopic systems which present long-range correlations: The behaviour at some position X depends on the current state of another far position Y . If one slightly “shakes”, or perturbs, the system at Y , an observer at X feels the effect of the shake in spite of the long distance X - Y . Indeed, as the distance increases, the intensity of the effects of the perturbation decays, but not according to the normal exponential decay, for which there is a characteristic correlation length beyond which correlations can be neglected. Within critical systems, instead, the decay normally follows a power-law, lacking any characteristic length: no matter how distant X is from Y , the effects of the perturbation cannot be neglected. All length scales are equally important. The reductionist approach of taking only a small, localised piece of the system clearly does not work: critical systems must be studied as a whole. Outside equilibrium, in most cases, the power-law decays responsible for the long-range spatial correlations also appear defining the time dependence of the various quantities of interest: they produce long-memory effects, small contingencies occurred a long time ago can be determinant for the present situation of the critical system. All time scales are equally important. These features turn it very difficult to model a critical system through simple space-time differential equations.

On the other hand, the length and time scale-free behaviour of critical phenomena provides an interesting feature: Both the microscopic details and the short-term dynamics are not crucial for the long-range and long-term evolution of the system under study. Only some general characteristics as the spatial dimension and symmetries matter. Systems sharing the same spatial dimension and

symmetries fall into the same universality class, in spite of the big differences in what concerns the microscopic and short-term behaviour of each one. For critical systems in equilibrium, this universality concept was already well understood through the Wilson's renormalisation group. An equivalent general theory for systems out of equilibrium is still lacking, but the evidences of universal time dependent behaviour joining together completely different systems are ubiquitous. Universality allows us to model complicated real systems by toy models belonging to the same universality class, simplifying a lot the study of these systems. Even so, due to the long-range and long-memory features, one cannot hope to solve the toy model by the reductionist paradigm, by following only a small piece of the system during a small interval of time. The population dynamics simulation approach appears instead as the most important instrument for these studies.

This book shows some examples of critical dynamic systems studied through computer simulations. They belong to different fields, not just Physics, and are connected by two very general features. First, they are critical, presenting long-range correlations and long-term memories. Second, they are modelled by simple rules one can easily program on a computer, turning it possible to follow in seconds what corresponds to centuries of the real system under study.

We wanted to avoid, also because of the way references had to be put in this edition, to present a book which would mainly be a list of references surrounded by little text. Thus, not only have we selected a few fields of interdisciplinary computer simulations with which we are more familiar, but also chose to reference within these fields papers which we feel are the most important, as seen both from today's perspective and from our restricted interests and knowledge. We are aware of the fact that important papers will for sure be missing from our list of references, and we apologize to the reader and to the authors for that mostly unwanted omission.

We start in Chapter 2 with general principles of evolution, and then apply them to biology in Chapters 3 (ageing) and 4 (speciation). Then comes the presently fashionable field of languages (Chapter 5) and the related one of sociophysics (Chapter 6). Finally, Chapter 7 gives applications to earthquakes. Our summary in Chapter 8 tries to point out the similarity in the methods used in the previous chapters. An appendix, Chapter 9, lists and explains selected complete computer programs, written in Fortran – for the desperation of half the authors and as an early example of Galam conservatism model explained in Section 6.3.1.

Evolution

The word “evolution” is directly linked with time. Something which evolves is not static, it varies as time goes by. A variable quantity x describing such a dynamic system is a function of time, $x(t)$. The speed of its variation is measured by the first derivative dx/dt of this function, the acceleration by the second derivative d^2x/dt^2 , and so on. The canonical way to study this kind of problems is through the so-called differential equations, i.e., mathematical relations linking x with dx/dt , d^2x/dt^2 , etc.

A famous example is Newton’s law

$$m \frac{d^2x}{dt^2} = F(x)$$

which describes the movement of a particle with mass m along the X axis. $F(x)$ is the external force which drives the movement.

Another famous example is the Schrödinger equation

$$i\hbar \frac{d|\psi\rangle}{dt} = H|\psi\rangle$$

which tells us how the state $|\psi\rangle$ of a quantum system evolves in time. H is the Hamiltonian operator for this system, essentially its energy. \hbar is the Planck constant, and $i = \sqrt{-1}$ is the imaginary unit for complex numbers (nothing to do with complexity).

Diffusion also obeys a differential equation

$$\frac{\partial \rho}{\partial t} = D \nabla^2 \rho$$

where $\rho(\vec{r}, t)$ represents the local density of the diffusing material at position $\vec{r} = (x, y, z)$ and time t . The Laplacian operator ∇^2 sums up the second derivatives with respect to x , y and z , and D is the diffusion coefficient. This problem was studied by Einstein, in one of his five famous papers published in 1905, “Einstein’s Miraculous Year” (Einstein, 1998). Now, exactly one century later, UN and UNESCO commemorate the “World Year of Physics, WYP2005”, with a lot of events all over the world. Diffusion describes, for instance, how an ink drop